

4-Methoxybenzoic acid, 8-chlorooctyl ester

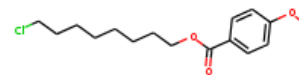
InChI: InChI=1S/C16H23ClO3/c1-19-15-10-8-14(9-11-15)16(18)20-13-7-5-3-2-4-6-12-17/h8-11H,2-7,12-13H2,1H3

InChI Key: NBGBVTBBAOFRQV-UHFFFAOYSA-N

Formula: C16H23ClO3

SMILES: COc1ccc(C(=O)OCCCCCCCCCl)cc1

Molecular Weight: 298.80



Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	-164.23	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-541.27	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	39.02	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	70.10	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	4.431		Crippen Method
P_c	1671.43	kPa	Joback Method
T_{boil}	733.28	K	Joback Method
T_c	932.17	K	Joback Method
T_{fus}	433.33	K	Joback Method
V_c	0.914	m ³ /kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	657.83	J/mol×K	733.28	Joback Method
η	0.0000844	Paxs	733.28	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C16H23ClO3/c1-19-15-10-8-14\(9-11-15\)16\(18\)20-13-7-5-3-2-4-6-12-17/h8-11H,2-7,12-13H2,1H3](http://webbook.nist.gov/cgi/inchi/InChI=1S/C16H23ClO3/c1-19-15-10-8-14(9-11-15)16(18)20-13-7-5-3-2-4-6-12-17/h8-11H,2-7,12-13H2,1H3)

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

$C_{p, \text{gas}}$: Ideal gas heat capacity (J/mol×K).

η : Dynamic viscosity (Pa×s).

$\Delta_f G^\circ$: Standard Gibbs free energy of formation (kJ/mol).

$\Delta_f H^\circ_{\text{gas}}$: Enthalpy of formation at standard conditions (kJ/mol).

$\Delta_{\text{fus}} H^\circ$: Enthalpy of fusion at standard conditions (kJ/mol).

$\Delta_{\text{vap}} H^\circ$: Enthalpy of vaporization at standard conditions (kJ/mol).

$\log P_{\text{oct/wat}}$: Octanol/Water partition coefficient .

P_c : Critical Pressure (kPa).

T_{boil} : Normal Boiling Point Temperature (K).

T_c : Critical Temperature (K).

T_{fus} : Normal melting (fusion) point (K).

V_c : Critical Volume (m³/kg-mol).

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